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L1 2710 S ISOTOP? (1A) DILUT? (3A) MASS SPECTRO? OR IDMS OR SIDMS
L2 128 S L1 AND (AUTOMAT? OR ONLINE OR INLINE OR REAL TIME OR ONSTREAM)
L3 75 S L1 AND (PROCESS? OR QUALITY) (4A) (CONTROL? OR MONITOR?)
L4 162 S L2-3 NOT PY>2001

=> d bib,ab 1-162 14

(L4) ANSWER 9 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 136:160546 CA
TI The analysis of environmental metal speciation using LC-MS
AU Harrington, Chris F.
CS De Montfort University, Leicester, UK
SO LC-GC Europe (2000), 13(6), 420,422,424,426-427
AB The main anal. points of importance that must be considered during the anal. of metal speciation in 2 different environmental situations are discussed. The use of a combined mass spectrometry approach, using elemental and mol. techniques, was shown to improve the validation of the speciation of metals. The improvements in the precision attainable for the measurement of environmentally and toxicol. important organometallic compds. by an **online IDMS** (isotope diln. MS) approach are also demonstrated.

(L4) ANSWER 12 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 136:84847 CA
TI Stable **isotope dilution** assay **mass spectrometry** in flavour research: internal standard and calibration issues
AU Fay, L. B.; Metairon, S.; Lin, J.; Blank, I.
CS Nestle Research Centre, Nestec Ltd., Lausanne, 1000, Switz.
SO Frontiers of Flavour Science, [Proceedings of the Weurman Flavour Research Symposium], 9th, Freising, Germany, June 22-25, 1999 (2000), Meeting Date 1999, 125-131. Editor(s): Schieberle, Peter; Engel, Karl-Heinz. Publisher: Deutsche Forschungsanstalt fuer Lebensmittelchemie, Garching, Germany.
AB Mass spectrometry is widely used in flavor research to quantify compds. by using isotopically labeled internal stds. However, equimolar amts. of different mols. do not give equal instrumental responses. Therefore, calibration of the mass spectrometer is needed prior to any sample quantification. If the mass of the internal std. differs from that of the analyte by more than 3 Da, the calibration curve is linear. If this mass difference is lower, a second-order curve is obtained that can be linearized by applying various math. treatments. We tested a no. of linearization techniques and recommend the method that uses isotopic enrichment calcn. to **control the quality** of the mass spectrometer's calibration.

(L4) ANSWER 13 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 136:84846 CA

TI On-line HRGC-IRMS determination of $\delta^{13}\text{C}$ and $\delta^{18}\text{O}$ values of flavour compounds - on the way to multi-element isotope ratio analysis for authenticity assessment

AU Hor, K.; Ruff, C.; Weckerle, B.; Konig, T.; Schreier, P.

CS University of Wurzburg, Wurzburg, 97074, Germany

SO Frontiers of Flavour Science, [Proceedings of the Weurman Flavour Research Symposium], 9th, Freising, Germany, June 22-25, 1999 (2000), Meeting Date 1999, 107-110. Editor(s): Schieberle, Peter; Engel, Karl-Heinz. Publisher: Deutsche Forschungsanstalt fuer Lebensmittelchemie, Garching, Germany.

AB For the first time, **online** HRGC-IRMS detd. $\delta^{18}\text{OSMOW}$ values of two selected flavor compds., i.e. γ -decalactone and (Z)-3-hexenol are represented. The data show the potential of addnl. isotopic information for authenticity assessment of the origin of flavor. Correlation of $\delta^{18}\text{OSMOW}$ with $\delta^{13}\text{CPDB}$ data is a first step for future multi-element HRGC-IRMS anal., in which $\delta^{13}\text{CPDB}$, $\delta^{18}\text{OSMOW}$ and $\delta^{2}\text{HSMOW}$ will be included.

~~AN~~ ANSWER 17 OF 162 CA COPYRIGHT 2004 ACS on STN
135:251034 CA

TI Isotope dilution analysis for trace metal speciation

AU Garcia Alonso, J. Ignacio; Ruiz Encinar, Jorge; Sariego Muniz, Cristina; Marchante Gayon, J. Manuel; Sanz Medel, Alfredo

CS Department of Physical and Analytical Chemistry, University of Oviedo, Oviedo, 33006, Spain

SO Special Publication - Royal Society of Chemistry (2001), 267, 327-346

AB Recent advances in the authors' lab. on isotope diln. anal. for trace metal speciation using both species-specific and species-unspecific spiking are discussed. First, the authors will report on the application of isotope diln. anal. **online** with Fast Protein Liq. Chromatog. (FPLC) coupled to a double focusing ICP-MS (ELEMENT, Finnigan MAT) for the speciation of Fe, Cu and Zn in human serum. For this anal. the species-unspecific spike mode is suitable due to the complexity of the structure of the main proteins binding Fe (transferrin), Cu (ceruloplasmin) and Zn (albumin) in human serum. Secondly, the use of a ^{119}Sn enriched mono, di- and tributyltin spike for the accurate detn. of all three Sn species in sediments is described.

L4 ANSWER 26 OF 162 CA COPYRIGHT 2004 ACS on STN
134:90193 CA

TI Isotope dilution and sampling factors of the quality assurance and TQM of environmental analysis

AU Macasek, F.

CS Department of Nuclear Chemistry. Faculty of Natural Sciences, Comenius University, Bratislava, SK-84215, Slovakia

SO Journal of Radioanalytical and Nuclear Chemistry (2000), 246(3), 709-718

AB A review, with 28 refs., is given. Sampling and preparatory treatment of environmental objects is discussed from the view of their

information content, functional speciation of the pollutant, statistical distribution treatment and uncertainty assessment. During homogenization of large samples, a substantial information may be lost and validity of environmental information becomes vague. Isotope diln. anal. (IDA) is discussed as the most valuable tool for both validity of anal. and evaluation of samples variance. Data collection for a nonparametric statistical treatment of series of nonrepresentative subsamples, and physicochem. speciation of analyte may actually better fulfill criteria of similarity and representativeness. Large samples are often required due to detection limits of anal., but the representativeness of environmental samples should be understood not only by the mean analyte concn., but also by its spatial and time variance. Hence, heuristic anal. scenarios and interpretation of results must be designed by cooperation of environmentalists and anal. chemists.

ANSWER 28 OF 162 CA COPYRIGHT 2004 ACS on STN
133:232176 CA

TI Uncertainty calculations for amount of chemical substance measurements performed by means of **isotope dilution mass spectrometry** as part of the PERM project

AU Dobney, A.; Klinkenberg, H.; Souren, F.; Van Borm, W.

CS DSM Research, Geleen, 6160 MD, Neth.

SO Analytica Chimica Acta (2000), 420(1), 89-94

AB DSM Research was a partner in the certification round of a project, organized under the auspices of the European Commission's Fourth Framework Stds. Measurement and Testing Program, to produce two polyethylene ref. materials. The project, entitled Polymer Elemental Ref. Material (PERM SMT4-CT95 3024) required the detn. of the concns. of Cr, Cd, Hg and Pb in two polyethylene materials which were identified as PERM T3 high and PERM T3 low. Anal. was accomplished by an inhouse developed '**online**' **isotope diln. mass spectrometry** (**IDMS**) method using quadrupole ICPMS. This paper focuses on calcg. the uncertainty of these **IDMS** measurements. Since all anal. measurement results have an uncertainty assocd. with them, it is considered best practice, within metrol. circles, to state an uncertainty, as an integral part of any measurement result. The authors used a Monte Carlo simulation to est. the uncertainties assocd. with the measured concns. of Cr, Cd, Hg and Pb in the PERM T3 (high and low) materials. By participating in an interlab. exercise the authors were able to compare the authors' results with those of other labs. that used both classical **IDMS** and other techniques. The authors' results agreed with the overall mean of all participating labs., within stated uncertainties. Also the authors' uncertainties derived from Monte Carlo simulation were of the same magnitude as those obtained for the classical **IDMS** approach.

ANSWER 29 OF 162 CA COPYRIGHT 2004 ACS on STN
133:116988 CA

TI Assay for free and total carnitine in human plasma using tandem mass spectrometry

AU Stevens, Robert D.; Hillman, Steven L.; Worthy, Steven; Sanders, Doris; Millington, David S.
CS Duke University Medical Center, Research Triangle Park, NC, 27709, USA
SO Clinical Chemistry (Washington, D. C.) (2000), 46(5), 727-729
AB The authors have developed a new carnitine assay method based on **isotope-diln.** tandem **mass spectrometry** (TMS). The method is inherently more straightforward and accurate than previously reported methods, primarily because it has abs. mol. specificity, uses an isotope-labeled internal std. to compensate for any losses or variance resulting from the sample prepn., and has no known chem. interference. Aliquots of the samples (20 μ L) were injected directly into the electrospray ion source of a tandem mass spectrometer and data were acquired using a precursor ion scan of m/z 85 product ions over the range m/z 160-210. The spectra were acquired in the multichannel acquisition mode with a scan time of 1 s at a collision cell argon pressure of 0.22 Pa. During the acquisition, the flow rate was reduced to 30 μ L/min; under these conditions, each sample anal. took ~2.0 min. The within-day and between-day results for replicate analyses are well within accepted limits. **Quality control** (QC) values for a previously analyzed patient sample replicated to within 5% on consecutive assays. These results are a major improvement over the values measured by the Cobas method, which had CVs that typically ranged from -10% to 22% for QC samples. The results for 76 patient samples assayed by the Cobas spectrophotometric method were compared with those from the new TMS assay. There was good correlation between the two methods for both free and total carnitine detns.: free carnitine, $y = 1.04 + 1.017x$; $Sy|x = 3.49$; $r = 0.941$; total carnitine, $y = 1.89 + 0.974x$; $Sy|x = 4.77$; $r = 0.913$. The method was extended to include measurements of acetyl carnitine by adding a mixt. of labeled carnitines to plasma and calcg. concns. from calibration curves for free, acetyl, and total carnitine.

L4

ANSWER 34 OF 162 CA COPYRIGHT 2004 ACS on STN
131:211118 CA

AN Validation of new instrumentation for **isotope dilution mass spectrometric** determination of organic serum analytes
AU Ellerbe, P.; Phinney, C. S.; Sniegoski, L. T.; Welch, M. J.
CS National Institute of Standards and Technology, Gaithersburg, MD, 20899-0001, USA
SO Journal of Research of the National Institute of Standards and Technology (1999), 104(2), 141-145
AB A major activity in the 20 yr collaboration between the Anal. Chem. Division at NIST and the College of American Pathologists (CAP) has been the development of highly accurate and precise "definitive" methods for important clin. analytes in human serum. Definitive methods for org. analytes use **isotope diln./gas chromatog./mass spectrometry** and require a mass spectrometer capable of making highly precise measurements of the ratio between the ion intensities of a characteristic ion from the analyte of interest and its stable-isotope-labeled analog. Recently, the mass spectrometer used for 20 yr for definitive method development and measurements was replaced with a

main one

modern instrument capable of **automated** operation, with accompanying gains in convenience and sample throughput. Switching to the new instrument required modifications of measurement protocols, acceptance criteria, and ratio calcns. with background corrections to go along with **automated** instrument operation. Results demonstrated that the two instruments gave comparable results for measurements of both urea and cholesterol in samples from various serum-based Std. Ref. Materials [SRMs] and College of American Pathologists materials.

L4 ANSWER 35 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 131:208242 CA
TI Determination of cadmium in environmental and biological reference materials using isotope dilution analysis with a double focusing ICP-MS: a comparison with quadrupole ICP-MS
AU Valles Mota, J. Pablo; Ruiz Encinar, Jorge; Fernandez de la Campa, M. Rosario; Garcia Alonso, J. Ignacio; Sanz-Medel, Alfredo
CS Department of Physical and Analytical Chemistry, University of Oviedo, Oviedo, 33006, Spain
SO Journal of Analytical Atomic Spectrometry (1999), 14(9), 1467-1473
AB *Adapted* A detailed examn. of the performance of a double focusing (DF) sector field ICP-MS (Element, Finnigan MAT) for the ID-ICP-MS detn. of Cd in biol. and environmental samples is described and compared with a quadrupole-based instrument (HP4500, Hewlett Packard). Exptl. parameters governing the instrumental precision and accuracy for isotope ratio measurements of Cd in the DF-ICP-MS are 1st characterized. Systematic errors, including dead time, mass bias effects and spectroscopic interferences, can be easily cor. in the two instruments studied. Detector dead time has only to be taken into account using the DF-ICP-MS. Typical isotope ratio precisions of 0.2-0.3% can be obtained routinely with both instruments. However, the precision of the measurements in the DF-ICP-MS can be improved (<0.1%) by increasing the no. of scans. Also, for very low Cd concns. the DF-ICP-MS at low resoln. setting (R = 300) can provide better isotope ratio precision than the quadrupole ICP-MS because of its higher sensitivity. Both ICP-MS instruments were successfully applied to the detn. of very low levels of Cd by ID-ICP-MS (by both conventional and **online** ID modes) in biol. and environmental certified ref. materials, including Freeze-Dried Urine NIST SRM-2670, Horse Kidney IAEA H-8, Lichens BCR TP-25, Marine Sediment PACS-1 and Riverine water SLRS-3. Combined uncertainty assocd. with the detns. is addressed.

L4 ANSWER 36 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 131:110605 CA
TI A critical comparison of **online** coupling IC-ICP- (AES, MS) with competing analytical methods for ultra trace analysis of microelectronic materials
AU Seubert, Andreas
CS Institute Inorganic Chemistry, Univ. Hannover, Hannover, D-30167, Germany
SO Fresenius' Journal of Analytical Chemistry (1999), 364(5), 404-409
AB **Online** coupling of ion chromatog. and at. spectrometry (IC-ICP- (AES,

MS)) are compared to ref. methods and other competing methods for ultra trace characterization of solid microelectronic materials. The comparison is based on anal. data gained for well characterized samples by a no. of different labs. The matrixes used for comparison are Mo, Mo-oxide, MoSix, W, W-oxide, WSix, metallic As, red P, and Re. The analyte elements accessible by IC-ICP-(AES, MS) and with ref. values for at least 1 other method are Ag, Al, Ba, Ca, Cd, Cr, Co, Cu, Fe, K, Mg, Mn, Na, Ni, Ti, Tl, Th, U, and Zn. The agreement of results of IC-ICP-(AES, MS) with those of **isotope diln. mass spectrometry (IDMS)** and radiochem. activation analyses (RNAA) shows good accuracy for most elements and some contamination problems with ubiquitous elements. A correlation of IC-ICP-(AES, MS) and GDMS results is doubtless, but the discrepancies are rather high. As further technique ETV-ICP-MS is compared, whose results are in reasonable agreement with IC-ICP-(AES, MS). Details on some new applications as well as of some new methodol. enhancements of **online** coupling IC-ICP(AES, MS) for the matrixes As and P were included.

L4 ANSWER 43 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 130:191097 CA
TI Determination of cadmium in biological and environmental materials by **isotope dilution** inductively coupled plasma **mass spectrometry**: effect of flow sample introduction methods
AU Valles Mota, J. Pablo; Fernandez de la Campa, M. Rosario; Garcia Alonso, J. Ignacio; Sanz-Medel, Alfredo
CS Department of Physical and Analytical Chemistry, University of Oviedo, Oviedo, 33006, Spain
SO Journal of Analytical Atomic Spectrometry (1999), 14(2), 113-120
AB Exptl. parameters governing the instrumental precision and accuracy for isotope ratio measurements of cadmium in ICP-MS, including sampling time, mass bias, detector dead-time and spectroscopic interferences, were 1st characterized. The precision achieved for the isotope ratio detn. of Cd was ~0.2% (relative std. deviation for n = 5) both for 111:112 and 111:114 ratios. Two alternative flow approaches for the detn. of ultratrace concns. of cadmium by isotope diln. (ID) were explored and compared with the more conventional ID methodol.: 1st, **online** mixing of the sample soln. with the spike soln. just before the ICP-MS nebulizer using a peristaltic pump and, 2nd, the generation of volatile cadmium species using sodium tetraethylborate by merging zones flow injection ICP-MS. The three approaches were successfully applied to the detn. of ultratrace levels of cadmium in biol. and environmental certified ref. materials (NIST SRM 2670 Freeze-Dried Urine, IAEA H-8 Horse Kidney, BCR TP-25 Lichens, PACS-1 Marine Sediment and SLRS-3 Riverine Water). The **online** ID method proved to be the most convenient for the detn. of cadmium in such samples because it is fast, provides similar results to those of conventional ID and requires less sample prepns.

Relevant

ANSWER 46 OF 162 CA COPYRIGHT 2004 ACS on STN
130:41105 CA

TI Laboratory and natural diffusivity calibrations for apatite (U-Th)/He

thermochronometry
AU Farley, K. A.; House, M. A.; Kohn, B. P.
CS Division of Geological and Planetary Sciences, California Institute of Technology, Pasadena, CA, 91125, USA
SO Mineralogical Magazine (1998), 62A(Pt. 1), 436-437
AB The He diffusion behavior of gem-quality and more typical apatites was studied by using a fully **automated isotope diln. quadrupole mass spectrometry** system. Results of expts. demonstrate good reproducibility and confirm previous measurements by R. A. Wolf et al. (1996) of the He closure temp. ($tc \approx 75^\circ$) of Durango fluorapatite. Most of the other apatites analyzed yielded linear Arrhenius plots and tc values in the range 70-80°. However, some apatites exhibit a zig-zag pattern in which the apparent diffusivity at a given temp. increases as the temp. proceeds. Such behavior is attributed to nonuniform initial concn. of the He in the mineral. To confirm that lab. diffusivity data can be extrapolated to conditions relevant in nature, He ages of apatites from borehole sedimentary and igneous rocks were detd. and plotted against borehole temp. The age-temp. profiles are generally consistent with extrapolations of lab. diffusivity data. Also, from the radiogenic prodn.-diffusion equation, it is shown that isothermal apatites will approach a steady-state age where ingrowth balances diffusion.

LM ANSWER 48 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 129:117156 CA
TI Accurate determination of element species by **online** coupling of chromatographic systems with ICP-MS using isotope dilution technique
AU Heumann, Klaus G.; Gallus, Stefan M.; Radlinger, Gunther; Vogl, Jochen
CS Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg-University Mainz, Mainz, D-55099, Germany
SO Spectrochimica Acta, Part B: Atomic Spectroscopy (1998), 53B(2), 273-287
AB The instrumental design for coupling different liq. chromatog. systems such as ion, reversed phase, and size exclusion chromatog. as well as capillary gas chromatog. with ICP-MS for the detn. of element species is described. For accurate analyses obtaining '**real time**' concns. of chromatog. peaks, the **isotope diln. mass spectrometric (IDMS)** technique is applied. Two different spiking modes are possible, one using species-specific and another one using species-unspecific spike solns. of isotope-enriched labeled compds. The species-specific mode is only possible for element species well defined in their structure and compn., for example iodate or selenite, whereas the species-unspecific mode must be applied in all cases where the structure and compn. of the species is unknown, for example, for metal complexes with humic substances. For accurate detns. by the isotope diln. technique the mass discrimination effect must also be taken into account. Iodate, iodide and organoiodine species, including those of humic substances, were analyzed in mineral, drinking and environmental H₂O samples by coupling different liq. chromatog. methods with ICP-**IDMS**. Heavy metal complexes with humic substances in H₂O samples of different origin were characterized by size exclusion/ICP-**IDMS**. The possibilities of detg.

different environmental Se species are discussed and the results for the anal. of selenite and selenate, which was carried out by GC/ICP-IDMS after converting these species into a volatile piazselenol compd., are presented.

L4 ANSWER 50 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 129:14108 CA
TI Direct determination of urinary iodine by inductively coupled plasma mass spectrometry using isotope dilution with iodine-129
AU Haldimann, Max; Zimmerli, Bernhard; Als, Claudine; Gerber, Hans
CS Section of Food Chemistry and Analysis, Swiss Federal Office of Public Health, Division of Food Science, Bern, 3003, Switz.
SO Clinical Chemistry (Washington, D. C.) (1998), 44(4), 817-824
AB An inductively coupled mass spectrometric method was developed for the direct detn. of I in urine. The application of isotope diln. anal. with added 129I offers new possibilities for automatic and accurate detns. The sample prepn. consists of diln. with an NH3 soln. contg. 129I. The validation was made by comparison with the results obtained in another lab. by a spectrophotometric method based on the Sandell-Kolthoff reaction. Different regression models, including max. likelihood estn., were used to compare the methods. None of the models revealed anal. bias between the two methods. The urine samples analyzed for validation were from three persons previously exposed to an I bath and covered a concn. range of 0.2 to 2.8 μ mol/L. A detection limit of 0.02 μ mol/L, a within-run CV of 2.5%, and a between-run CV of 11.9% were estd. for the proposed method.

L4 ANSWER 51 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 129:1473 CA
TI A fast universal automated cleanup system for the isotope-dilution high-resolution mass spectrometric analysis of PCDDs, PCDFs, coplanar-PCBs, PCB congeners, and persistent pesticides from the same serum sample
AU DiPietro, E. S.; Lapeza, C. R., Jr.; Cash, T. P.; Turner, W. E.; Green, V. E.; Gill, J. B.; Patterson, D. G., Jr.
CS Dioxin Related Compounds Lab., Toxicology Branch, Div. Environmental Health Laboratory Science, Centers Disease Control Prevention, National Center Environmental Health, Atlanta, GA, 30341, USA
SO Organohalogen Compounds (1997), 31, 26-31
AB A new parallel automated sample cleanup app. was developed able to simultaneously process up to 10 serum sample exts. in <1 h. In addn. to the usual 22 polychlorinated dibenzo-p-dioxins, dibenzofurans, and non-ortho-substituted or coplanar polychlorinated biphenyls (PCB), the app. was used to collect ortho-substituted PCB and persistent pesticides in 2 sep. fractions during the same cleanup run. A new method was described to analyze 38 ortho-substituted PCB and 13 chlorinated persistent pesticides in human serum by high-resoln. GC / isotope diln. high-resoln. MS.

L4 ANSWER 54 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 128:222712 CA

TI Development of efficient safeguards destructive analysis procedures at NMCC-SAL
AU Hara, Shinji; Shinohara, Toshihisa; Hatakenaka, Teruo; Nidaira, Kazuo; Yasu, Syouzou
CS Nuclear Material Control Center Safeguards Analytical Laboratory, Shirakata, Japan
SO Nuclear Materials Management (1997), 26(2), 1278-1283
AB The U and Pu isotopic compns. and concns. of safeguards inspection samples are measured mainly by the **mass spectrometry** and **isotopic diln. mass spectrometry (IDMS)** at Safeguards Anal. Lab. of Nuclear Material Control Center (NMCC-SAL) in Japan. In these methods, chem. sepn. of U, Pu, Am and other interfering nuclides, and precise measurement of isotopic compns. are indispensable. The ion exchange procedure is used for the sepn., but it requires a lot of workload and long operation time to result in inefficient anal. procedures. For mass spectrometry, it generally takes about an hour for the measurement of one sample by the conventional method using bias collection factor (BCF). To improve the efficiency of anal., **automated** ion exchange sepn. unit was developed to reduce workload, and total evapn. mass spectrometry method was examd. to reduce measurement time. These methods are expected to be used at Rokkasyo Reprocessing Plant On Site Lab. (RRP-OSL) in future. This paper will describe the outline of these anal. procedures with emphasis on the performance of the **automated** ion exchange unit and total evapn. method, as well as their anal. results compared with conventional methods.

ANSWER 57 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 128:119284 CA
TI **Automated Online** Isotope Dilution Analysis with ICP-MS Using Sandwich Flow Injection
AU Specht, August A.; Beauchemin, Diane
CS Department of Chemistry, Queen's University, Kingston, ON, K7L 3N6, Can.
SO Analytical Chemistry (1998), 70(5), 1036-1040
AB An **automated** flow injection (FI) manifold is described to perform the addn. of isotopic spikes to aq. samples **online** with ICP-MS for isotope diln. (ID) anal. The manifold uses the sandwich technique (with the nested loop approach) to perform an injection of the isotopic spike soln. within a sample (or std.) plug, the resulting sample-spike-sample sequence being pushed toward the nebulizer by a 1% HNO₃ carrier. A std., which must contain one element not present in the spike soln. to allow the detn. of the dispersion coeff., must also be used to allow a reverse isotope diln. anal., as well as corrections for mass discrimination and/or spectroscopic interferences. Indeed, because the signals from the individual isotopes are monitored continuously, only one isotope free of spectroscopic interference is required for elements whose isotopic distribution does not vary in nature (two isotopes are still needed for the other elements), as a correction for the interference can be made by comparison with the signals from the std. Furthermore, this **automated** approach makes ID-ICP-MS a faster method and does not require any preliminary anal. of the sample because the

concn. profile resulting from FI allows the selection of the best isotopic ratio. It was successfully applied to the detn. of Mo in saline water.

Aden 15

L4 ANSWER 59 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 127:311257 CA
TI Determination of heavy metal complexes with humic substances by HPLC/ICP-MS coupling using **online** isotope dilution technique
AU Vogl, Jochen; Heumann, Klaus G.
CS Institute Inorganic Chemistry Analytical Chemistry, Johannes Gutenberg-University, Mainz, D-55099, Germany
SO Fresenius' Journal of Analytical Chemistry (1997), 359(4-5), 438-441
AB An **isotope diln. mass spectrometric (IDMS)** method has been developed for the simultaneous detn. of the complexes of 11 heavy metals (Ag, Cd, Cu, Mo, Ni, Pb, Tl, U, W, Zn, and Zr) with humic substances (HS) by coupling HPLC with ICP-MS and applying the **online** isotope diln. technique. The HPLC sepn. was carried out with size exclusion chromatog. This HPLC/ICP-IDMS method was applied to samples from a brown water, ground water, sewage and seepage water as well as for a sample contg. isolated fulvic acids. The total contents of heavy metals and of their complexes were analyzed in these samples with detection limits in the range of 5-110 ng/L. The anal. of heavy metal/HS complexes from the different waters resulted in characteristic fingerprints of the distribution pattern of heavy metals in the sepd. HS fractions. A comparison between the total heavy metal concns. and their portions bound to humic substances showed distinct differences for the various metals. Simultaneous ¹²C detection was used for the characterization of HS complexes not identified by UV detection and for the detn. of relative DOC concns. of chromatog. peaks.

ANSWER 62 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 127:103617 CA
TI A study of random and systematic errors for the determination of molybdenum by inductively coupled plasma **mass spectrometry** using **online isotope dilution** analysis
AU Marchante-Gayon, J. M.; Garcia Alonso, J. I.; Sanz-Medel, A.
CS Dep. Phys. and Analytical Chemistry, Faculty Chemistry, Univ. Oviedo, Oviedo, 33006, Spain
SO Special Publication - Royal Society of Chemistry (1997), 202(Plasma Source Mass Spectrometry), 85-94
AB Reverse isotope diln. anal. was applied for the detn. of the concn. of a ⁹⁵Mo enriched spike and the procedure was **automatized** using an auto sampler where natural Mo stds. and samples where alternatively mixed **online** with the spike soln. A new equation is proposed for the **online** mixing of samples and spike using the autosampler. The measurement of a natural Mo std. between the samples makes possible to perform isotope diln. anal. referring the results to the natural Mo std. regardless of the concn. of the spike. The effects of both systematic and random errors were examd. and the error theory was applied for the accurate detn. of Mo in biol. materials by ID-ICP-MS.

ANSWER 66 OF 162 CA COPYRIGHT 2004 ACS on STN
126:98532 CA
TI Determination of Environmental Lead Using Continuous-Flow Microwave Digestion **Isotope Dilution** Inductively Coupled Plasma **Mass Spectrometry**
AU Beary, Ellyn S.; Paulsen, Paul J.; Jassie, Lois B.; Fassett, J. D.
CS Chemical Science and Technology Laboratory, National Institute of Standards and Technology, Gaithersburg, MD, 20899, USA
SO Analytical Chemistry (1997), 69(4), 758-766
AB A com. flow-through microwave system was successfully applied as an alternative sample prep. procedure for lead detns. using isotope diln. inductively coupled plasma quadrupole mass spectrometry. Sample is introduced as a slurry and then injected into a carrier stream which is continually flowing through the system. As configured, the sample dissoln. is sequential, taking ~10 min/sample. This closed system is easy to use and produces low blanks, thus providing a viable alternative to the direct introduction of untreated samples, which can degrade anal. results. Leaves, air filters, urine, sludge, dust, and paint std. ref. materials previously certified for lead using **isotope diln. mass spectrometry (IDMS)** were used to evaluate the accuracy of this **automated** sample prep. device. Lead concns. in the nanograms to micrograms per g range were accurately detd. when compared with the certified value and previous **IDMS** results.

ANSWER 68 OF 162 CA COPYRIGHT 2004 ACS on STN
126:66530 CA
TI A combined volumetric verification procedure based on bubble-tube manometry and lutetium spike
AU Lemley, James R.; Suda, Sylvester; Keisch, Bernard; Belew, Wendell; Smith, David H.
CS Brookhaven National Laboratory, Upton, NY, 11973, USA
SO Nuclear Materials Management (1994), 23, 978-982
AB Bubble-tube manometry is the most accurate currently available method for precision volumetric measurements of solns. in process tanks contg. special nuclear materials. Bubble tubes installed in the accountability tank by the facility operator are instrumented with a precision pressure transducer and a programmable pneumatic multiplexing system. In a process-soln. measurement technique currently under development, a spike soln. contg. a known amt. of Lu is added to the accountability tank, appropriate measures are taken to homogenize the tank contents, and a sample of the homogenized soln. is analyzed by **isotopic diln. mass spectrometry**. Each method offers unique advantages when applied to independent verification of the special nuclear material content of process solns. for the purposes of international safeguards. The methods are compared with regard to attributes such as intrusiveness, authentication independent of the facility operator, value for process operations, suitability for continuous unattended **process monitoring**, tech. implementation challenges, accuracy, inspection effort and cost. A soln.-vol. verification procedure emphasizing the complementary aspects of both methods is proposed. Application to the important process-soln. measurement and verification needs in international safeguards is analyzed, and its advantages are

clearly identified.

L4 ANSWER 80 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 122:122085 CA
TI Elemental speciation with liquid chromatography-inductively coupled plasma **isotope dilution mass spectrometry**
AU Heumann, Klaus G.; Rottmann, L.; Vogl, J.
CS Inst. Inorg. Chem., Univ. Regensburg, Regensburg, D-93040, Germany
SO Journal of Analytical Atomic Spectrometry (1994), 9(12), 1351-5
AB For the detn. of elemental species, which normally exist at low concns. in the environment, coupling of liq. chromatog. systems with inductively coupled plasma mass spectrometry (ICP-MS) is a powerful method with respect to detection limit. However, accurate results are still a problem in trace analyses but can be obtained by the application of **isotope diln. mass spectrometry (IDMS)**. The developed LC-ICP-**IDMS** system consists of a HPLC pump, a sample injection valve, a sepn. column (different types of chromatog. sepn. systems, e.g., ion or size-exclusion chromatog., were used depending on the sepn. problem), a nondestructive detector (e.g. a UV detector) for simultaneous detn. of org. substances, and an element-specific ICP mass spectrometer. Isotope diln. is carried out by adding an isotopically enriched species-specific spike soln. to the sample prior to the sepn. step in the case of the detn. of well-defined species, or by continuous **online** introduction of a species-specific spiking method is demonstrated for the detn. of iodide and iodate in mineral H₂O using an ion chromatog. sepn. column. For example, iodate concns. at 0.5-20 ng mL⁻¹ could be detd. with relative std. deviations of ~2%. The species-unspecific spiking mode was used to det. heavy metal complexes with humic substances at a level of ~1 ng mL⁻¹ as well as organo-I species in the concn. range 0.7-1.4 ng mL⁻¹ in natural H₂O systems. The accuracy of speciation could be verified by comparing the total element concn. with the sum of the different elemental species.

L4 ANSWER 81 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 122:122048 CA
TI Development of an **online** isotope dilution technique with HPLC/ICP-MS for the accurate determination of elemental species
AU Rottmann, Lothar; Heumann, Klaus G.
CS Instiut fuer Anorganische Chemie, Universitaet Regensburg, Regensburg, D-93040, Germany
SO Fresenius' Journal of Analytical Chemistry (1994), 350(4-5), 221-7
AB An **online** isotope diln. technique was developed for use with a HPLC system (HPLC) coupled to an inductively coupled plasma mass spectrometer (ICP-MS). With this method it is possible to characterize elemental species at low concn. levels and to quantify them accurately. The possibilities of this method are shown using the samples of the detn. of the interactions of different mol. wt. fractions of dissolved org. matter (DOM) with copper and molybdenum in a natural water sample.

L4 ANSWER 94 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 119:33989 CA

TI The use of an enriched isotope as an on-line internal standard in inductively coupled plasma mass spectrometry: a reference method for a proposed determination of tellurium in industrial waste water by means of graphite furnace atomic absorption spectrometry
AU Klinkenberg, Huub; Beeren, Ton; Van Borm, Werner; van der Linden, Fons; Raets, Mich
CS Dep. PAC, DSM Res., Geleen, 6160, Neth.
SO Spectrochimica Acta, Part B: Atomic Spectroscopy (1993), 48B(5), 649-61
AB The continuous addn. of a soln. of an enriched ^{125}Te as internal std. is used in an **online isotope diln.** inductively coupled plasma **mass spectrometry** (ID-ICP-MS) anal. for the detn. of Te in industrial wastewater. The method has the precision and accuracy attainable with isotope diln. In order to check for possible polyat. interferences, 2 analyte isotopes (^{128}Te and ^{130}Te) were used. Isotopic ratios were converted into calibration graphs that are curved for both analyte isotopes. A formula is presented, with which the shape of a calibration graph can be calcd. beforehand. ICP-MS has been used as a ref. method for a proposed graphite furnace at. absorption spectrometry (GFAAS) procedure that uses the combination of Pd, Triton X-100 and H as matrix modifier. Only Triton X-100 could assure the uniform atomization of Te. Obviously, the particle size distribution of Pd is much more important than the dispersion of Pd particles in the graphite furnace. Forty-eight wastewater samples were analyzed. The GFAAS and ICP-MS results were compared as paired samples using a t-test on their differences. At a confidence level of 0.05, both methods gave identical results.

QD 95. A1 56

~~14~~ ANSWER 97 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 118:97384 CA
TI Rapid diagnosis of phenylketonuria by quantitative analysis for phenylalanine and tyrosine in neonatal blood spots by tandem mass spectrometry
AU Chace, Donald H.; Millington, David S.; Terada, Naoto; Kahler, Stephen G.; Roe, Charles R.; Hofman, Lindsay F.
CS Med. Cent., Duke Univ., Durham, NC, 27710, USA
SO Clinical Chemistry (Washington, DC, United States) (1993), 39(1), 66-71
AB A new method for quantifying specific amino acids in small vols. of plasma and whole blood has been developed. Based on **isotope-diln.** **tandem mass spectrometry**, the method takes only a few minutes to perform and requires minimal sample prep. The accurate assay of both phenylalanine and tyrosine in dried blood spots used for neonatal screening for phenylketonuria in North Carolina successfully differentiated infants who had been classified as normal, affected, and falsely pos. by current fluorometric methods. Because the mass-spectrometric method also recognizes other aminoacidemias simultaneously and is capable of **automation**, it represents a useful development toward a broad-spectrum neonatal screening method.

~~14~~ ANSWER 107 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 114:224904 CA

TI **Automated** analysis of stable isotopes of zinc, copper, iron, calcium and magnesium by thermal ionization **mass spectrometry** using double **isotope dilution** for tracer studies in humans
AU Turnlund, Judith R.; Keyes, William R.
CS West. Hum. Nutr. Res. Cent., Presidio of San Francisco, CA, 94129, USA
SO Journal of Micronutrient Analysis (1990), 7(2), 117-45
AB Methods were developed for **automated**, multiple collector detn. of isotopic ratios of Zn, Cu, Fe, Ca, and Mg using a magnetic sector, thermal ionization mass spectrometer. Most isotopic ratios were measured accurately with internal and external precision of 0.1% relative std. deviation or less. **Automated** anal. was much faster than nonautomated thermal ionization mass spectrometry (TIMS) anal. Use of the multiple collector improved precision and speed of anal. Isotopic ratios were detd. as accurately and precisely for minerals sepd. from fecal, urine and blood plasma samples as for pure ref. stds. Methods for collecting and purifying biol. samples, measuring isotopic ratios, correcting the ratios for fractionation, and calcg. enrichment, absorption and endogenous excretion into the gastrointestinal tract are reported. Data from anal. of fecal, urine and plasma samples following infusion and feeding of stable isotopes of Zn, Cu and Fe are reported. The data demonstrate that isotopic ratios and enrichments can be detd. reliably in human tracer studies.

L4
ANSWER 110 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 112:228753 CA
TI On-line isotope dilution and sample dilution by flow injection and inductively coupled plasma mass spectrometry
AU Viczian, Miklos; Lasztity, Alexandra; Wang, Xioaru; Barnes, Ramon M.
CS Dep. Chem., Univ. Massachusetts, Amherst, MA, 01003-0035, USA
SO Journal of Analytical Atomic Spectrometry (1990), 5(2), 125-33
AB A systematic investigation was made to demonstrate the applicability of a flow injection system for **online** isotope diln. and **online** sample diln., as obtained by merging the sample soln. with the spike soln. or with the diluent, resp. The effect of the sample to spike ratio on the precision and accuracy was examd., and the advantages and limitations of the proposed technique are demonstrated.

L4
ANSWER 111 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 112:190922 CA
TI Sample analysis by on-line **isotope dilution** inductively coupled plasma **mass spectrometry**
AU Lasztity, Alexandra; Viczian, Miklos; Wang, Xioaru; Barnes, Ramon M.
CS Dep. Chem., Univ. Massachusetts, Amherst, MA, 01003-0035, USA
SO Journal of Analytical Atomic Spectrometry (1989), 4(8), 761-6
AB An **online** isotope diln. technique was developed by coupling com. flow injection instruments with an inductively coupled plasma mass spectrometer. Application of the technique was demonstrated by the detn. of lead concns. in diverse std. ref. materials. The precision of the method, using optimum sample to spike ratios and a steady-state merging stream, is better than 1%. The approach simplifies sample prepn. and anal., and matrix effects have no influence on the detns.

~~N4~~ ANSWER 124 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 105:126349 CA
TI Automatic titration apparatus for isotope dilution mass spectral analysis
IN Ezawa, Naoya; Kato, Yutaka; Takada, Koichi; Kunikata, Michio; Kawamura, Hironobu
PA Hitachi, Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 3 pp.
PI JP 61013153 A2 19860121 JP 1984-133193 19840629
PRAI JP 1984-133193 19840629
AB An **automatic** titrn. app. is claimed which has controls to regulate the spiking of a sample during isotope diln. mass spectral anal. By **automating** the spiking process, a large no. of samples differing in isotopic compn. can be analyzed.

~~N4~~ ANSWER 133 OF 162 CA COPYRIGHT 2004 ACS on STN
~~AN~~ 100:95751 CA
TI Simultaneous determination of americium and plutonium in plutonium nitrate solutions
AU Rebagay, T. V.; Lee, R. S.; Huff, G. A.
CS Allied-Gen. Nucl. Serv., Barnwell, SC, USA
SO Nuclear Materials Management (1983), 12(Proc. Issue), 168-74
AB A method for the simultaneous detn. of Am and Pu in reprocessing solns. using an **automated** on-line concn. monitor was developed and evaluated. The quant. assays for Pu were based on the intensities of the characteristic gamma rays of ^{238}Pu , ^{239}Pu , ^{240}Pu , and ^{241}Pu in the 120 keV to 210 keV region of the soln. spectra. The assay peak for Am were the 59.5 keV and 125 keV lines of ^{241}Am . The method is capable of measuring Am (1-1500 ppm) in Pu (5-50 g/L) solns. with an accuracy better than $\pm 2\%$ using the 59.5 keV peak of ^{241}Am . The obsd. Am data were compared with those obtained by alpha spectrometry and the values derived from the calcd. ^{241}Am (125 keV)/ ^{239}Pu (129 keV) ratios of the test solns. An overall av. deviation of 1% for ^{239}Pu and 3% each for ^{238}Pu , ^{240}Pu , and ^{241}Pu from the mass spectrometry data was noted for the isotopic distribution of Pu. The elemental Pu abundances compared very well with those measured by **isotope diln. mass spectrometry** and controlled-potential coulometry.

L4 ANSWER 136 OF 162 CA COPYRIGHT 2004 ACS on STN
AN 98:209152 CA
TI Isotope-dilution analyses of the metallic elements
AU Chastagner, P.
CS Savannah River Lab., Du Pont de Nemours (E.I.) and Co., Aiken, SC, USA
SO Report (1982), DP-MS-82-76; Order No. DE83004924, 31 pp. Avail.: NTIS
From: Energy Res. Abstr. 1983, 8(6), Abstr. No. 12752
AB The **isotope-diln. mass spectroscopy (IDMS)** technique has proven to be a reliable, versatile anal. tool. Its applications seem to be limited only by the ingenuity of the investigator. Among its advantages are: small sample size; general applicability; precision and accuracy; dynamic range; simplified chem.; detn. is fixed at the time and place

of isotopic homogenization. The last listed item is esp. important for nuclear safeguards and processes where inventories are crit. **IDMS** is now a routine anal. technique in geochem. and nuclear labs., and in many environmental labs. Microgram and nanogram samples are normally used, frequently with **automatic** mass spectrometers, in many of these routine applications. More advanced techniques permit picogram and sub picogram samples to be analyzed, and spike to sample ratios can range from 1:1 to 1:1012 with detection limits at attogram levels for some elements.

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